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For quantum mechanics on a lattice the position (“particle number”) operator and the quasi-momentum (“phase”) operator obey canonical commutation relations (CCR) only on a *dense set* of the Hilbert space. We compare exact numerical results for a particle in simple potentials on the lattice with the expectations, when the CCR are assumed to be *strictly* obeyed. Only for sufficiently smooth eigenfunctions this leads to reasonable results. In the long time limit the use of the CCR can lead to a *qualitatively* wrong dynamics even if the initial state is in the dense set.

Since the pioneering work on quantization of the electromagnetic field, where Dirac¹ introduced a phase observable, supposedly conjugate to the number operator \mathcal{N} , there has been a long controversy whether a phase operator $\hat{\theta}$ can be constructed which obeys the canonical commutation relation (CCR) $[\mathcal{N}, \hat{\theta}] = i\hat{1}$. As there exist excellent reviews which address this question^{2,3} it is not necessary to give a detailed history of the various proposals. We want to point out that there are different types of “number operators” of importance. In quantum optics the eigenvalues of the particle number operator run from *zero* to infinity. For the case of fermions with a filled Dirac sea one often works with the number operator relative to the Dirac sea which has integer eigenvalues which run from minus infinity to plus infinity^{4–6}. A conceptually simple case where the number operator is of the form $\mathcal{N} = \sum_{-\infty}^{\infty} |n\rangle n \langle n|$ is (apart from the multiplicative factor of the lattice spacing a) the position operator \hat{x} for quantum mechanics on a one-dimensional *lattice*⁷. In this paper case we treat infinite lattices which corresponds to the simpler case of a number operator *not* bounded from below³, while the quantum optics scenario corresponds to a semi-infinite lattice.

Shortly after Dirac’s introduction of the phase operator Jordan⁸ gave an argument why the CCR $[\mathcal{N}, \hat{\theta}] = i\hat{1}$ cannot hold as an operator identity. This commutation relation would imply $[\sin \alpha \mathcal{N}, \hat{\theta}] = i\alpha \cos \alpha \mathcal{N}$. If one puts $\alpha = \pi$ this leads to a *contradiction* as $\sin \pi \mathcal{N}$ is zero because \mathcal{N} has integer eigenvalues, but $\cos \pi \mathcal{N}$ is nonzero. It is only possible to construct a canonical pair $(\mathcal{N}, \hat{\theta})$ on a *dense set* of the states of the Hilbert space^{9,10}. The question we want to address in this paper is if this fact is useful for typical applications in physics, where a Hamiltonian is given and one wants to solve the time-independent and (or) the time-dependent Schrödinger equation. An example where in this context the canonical commutation relation $[\mathcal{N}, \hat{\theta}] = i\hat{1}$ is generally assumed is in treatments of the Josephson Hamiltonian¹¹.

As a simple example we study the properties of a particle described by the Hamiltonian

$$H = - \sum_{m,n} (|m+n\rangle t_n \langle m| + H.c.) + \sum_m |m\rangle V_m \langle m|, \quad (1)$$

where the t_n are the hopping matrix elements and the V_m are the local potentials. For a constant potential the (improper) eigenstates are the Bloch states

$$|k\rangle = \sqrt{\frac{a}{2\pi}} \sum_m e^{iakm} |m\rangle, \quad (2)$$

with k in the first Brillouin zone $(-\pi/a, \pi/a]$. The Bloch states are normalized as $\langle k|k'\rangle = \delta(k-k')$. The “obvious” operator to replace the momentum operator (divided by \hbar) on the lattice is the quasi-momentum operator

$$\hat{k} = \int_{-\pi/a}^{\pi/a} |k\rangle k \langle k| dk. \quad (3)$$

In the position representation $\hat{\theta} \equiv a\hat{k}$ is just the infinite lattice version of the “phase operator” proposed independently by Garrison and Wong⁹ and Galindo¹⁰ for the semi-infinite case

$$\hat{\theta}|n\rangle = \sum_{m(\neq n)} \frac{(-1)^{m-n}}{i(m-n)} |m\rangle. \quad (4)$$

If one applies $\hat{x} = a\mathcal{N}$ to the states in Eq. (4) one sees that $\hat{x}\hat{\theta}|n\rangle$ is not an element of the Hilbert space l_2 , while $\hat{\theta}\hat{x}|n\rangle$ is. A straightforward formal calculation shows that \hat{x} and \hat{k} do *not* obey a CCR

$$[\hat{x}, \hat{k}] |n\rangle = -i \sum_{m(\neq n)} (-1)^{m-n} |m\rangle. \quad (5)$$

The correction term can be expressed in terms of the projection operator on the Bloch state $|\pi/a\rangle$ ¹²

$$[\hat{x}, \hat{k}] = i \left(\hat{1} - \frac{2\pi}{a} \left| \frac{\pi}{a} \right\rangle \left\langle \frac{\pi}{a} \right| \right). \quad (6)$$

For states $|\psi\rangle$ where the components $\psi_n \equiv \langle n|\psi\rangle$ obey the condition $S_\psi \equiv \sum_n (-1)^n \psi_n = 0$ the correction term vanishes. These states form a *dense set* of states of the Hilbert space l_2 ¹⁰. This condition is fulfilled when the components in position space are sufficiently smooth. If $\psi_n = f(an)$, where f is a differentiable function, the

operator $i\hat{k}$ for $a \rightarrow 0$ acts like the differential operator $d/d(an)$. Using Eq. (4) this can be seen by writing

$$\langle n | i\hat{k} | \psi \rangle = \sum_{j=1}^{\infty} \frac{(-1)^{j+1}}{ja} (\psi_{n+j} - \psi_{n-j}). \quad (7)$$

With the assumption on the function f made above the series on the right hand side (rhs) is approximately of the form $2(f'(an) - f'(an) + f'(an) - + \dots)$ which quickly converges to $f'(an)$. This can be best seen using the Euler transformation¹³ of the sum on the rhs of Eq. (7).

We next consider *functions* of the operator \hat{k} . For integer n the exponential functions

$$e^{-ina\hat{k}} = \sum_m |m+n\rangle \langle m| \equiv \hat{T}_n \quad (8)$$

are just the discrete translation operators. Using the site representation one easily shows the commutation relation $[\hat{x}, e^{-ina\hat{k}}] = ane^{-ina\hat{k}}$, which also can be “derived” assuming the CCR. The latter incorrect derivation could also be performed if n is replaced by an arbitrary real number. But then the above result no longer holds, i.e. the use of the CCR gives a wrong answer. In the following we also use the operator \hat{k}^2 . Its matrix elements in the position representation are given by

$$a^2 \langle m | \hat{k}^2 | n \rangle = \frac{\pi^2}{3} \delta_{mn} + 2 \frac{(-1)^{m-n}}{(m-n)^2} (1 - \delta_{mn}). \quad (9)$$

Therefore the operator $\hat{k}^2/2$ has the form of the first term on the rhs of Eq. (1) with $t_0 = -\pi^2/(6a^2)$ and $t_n = (-1)^{n+1}/(an)^2$. The corresponding energy eigenvalues $\epsilon_k = -t_0 - 2 \sum_{n \geq 1} t_n \cos(akn)$ are just the well known Fourier series which corresponds to the periodically continued parabola arcs. In the following we mainly work with the Hamiltonian $H = \hat{k}^2/2 + V(\hat{x})$, which is a special case of Eq. (1).

We examine, if *assuming* the strict validity of the CCR $[\hat{x}, \hat{k}] = i\hat{1}$ can be useful in the description of a particle governed by such a Hamiltonian by comparison with exact results. We study the eigenvalue problem as well as solutions to the time dependent Schrödinger equation. Only for those eigenstates $|\psi_E\rangle$ which approximately fulfill $\langle \pi/a | \psi_E \rangle = 0$ we can expect the assumption $[\hat{x}, \hat{k}] = i\hat{1}$ to be useful.

We begin with the *harmonic oscillator on the lattice* $H = \hat{k}^2/2 + c\hat{x}^2/2$. The Josephson Hamiltonian in its most simple form¹¹ corresponds to a quadratic potential but with a kinetic energy \hat{T}_{kin} with nearest neighbour hopping $(\hat{1} - \cos a\hat{k})/a^2 = [\hat{1} - (T_1 + T_{-1})/2]/a^2$ for $a = 1$. We present results for both types of the kinetic energy and explicitly mention when $\hat{T}_{kin} = \hat{k}^2/2$ is *not* used. The exact solution can be obtained numerically by diagonalizing a sufficiently large matrix. The expectations from assuming the CCR $[\hat{x}, \hat{k}] = i\hat{1}$ are obvious if one introduces the usual ladder operators⁷ and

determines the eigenvalue spectrum purely algebraically, which yields $E_n = \sqrt{c}(n + 1/2)$. If we further assume the expectation value of the potential energy to be half the energy eigenvalue as in the continuum limit it follows that the the wave function $\psi_m^{(n)}$ approximately extends from $-(n/\sqrt{c})^{1/2}$ to $(n/\sqrt{c})^{1/2}$. The mean separation of the nodes of the corresponding wave function in the continuum is therefore given by $2/\sqrt{nc^{1/2}}$. The smoothness assumption which is necessary for the CCR to be approximately valid certainly breaks down, when this separation becomes of the order of the lattice constant a . One therefore expects the equidistant energy spectrum of the harmonic oscillator in the continuum to be approximately valid for quantum numbers n smaller than $b/\sqrt{a^4 c}$ where b is of order unity. The exact numerical results for the lattice model are shown in Fig. 1.

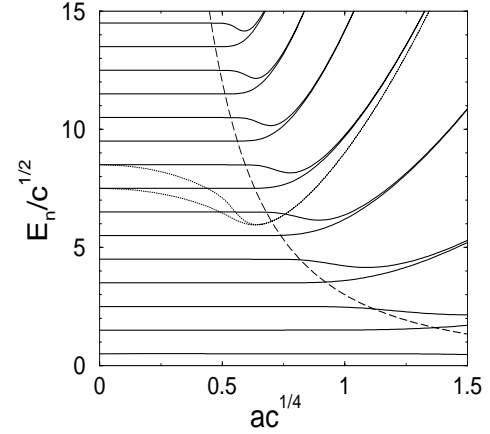


FIG. 1. Normalized energy eigenvalues of the harmonic oscillator on the lattice as a function of $ac^{1/4}$. Below the dashed line $3/(ac^{1/4})^2$ explained in the text one approximately recovers the eigenvalue spectrum of the continuum limit. The dotted line shows two eigenvalues for the kinetic energy $(\hat{1} - \cos a\hat{k})/a^2$.

The dashed line shows the criterion just derived for $b = 3$. Above this line there are strong deviations from the equidistant spectrum, in fact pairs of eigenvalues become almost degenerate. A simple explanation for this observation will be given later. For comparison we also show two eigenvalues for the nearest neighbour kinetic energy $(\hat{1} - \cos a\hat{k})/a^2$ which for small enough values of $ac^{1/4}$ are expected to form the same equidistant spectrum. As shown the results deviate from $E_n = \sqrt{c}(n + 1/2)$ already for smaller values of $ac^{1/4}$ and the almost degeneracy of the eigenvalue pair occurs already for a smaller value of $ac^{1/4}$ compared to the long range hopping. Fig. 2 shows the behaviour of the absolute value of the overlap $S_n \equiv \sum_m (-1)^m \psi_m^{(n)}$ as a function of the quantum number n for the even parity states. The values of n where S_n starts to become “nonzero” agree very well with expectation from the argument using the number of nodes.

In order to understand the spectrum in the upper right corner of Fig. 1 it is useful to first treat the case of a *linear* potential described by the Hamiltonian $H = \hat{k}^2/2 - F\hat{x}$. For such a potential the energy eigenvalue spectrum for the lattice model is known to be completely different from the continuum limit. It consists of an equidistant “Wannier-Stark”-ladder¹⁴, while the spectrum is purely continuous for the continuum case. This can easily be understood using the translation operators \hat{T}_n defined in Eq. (8) which obey the simple commutation relation $[\hat{T}_n, H] = anF\hat{T}_n$. After one localized eigenstate $|E_0\rangle$ with eigenvalue E_0 is shown to exist¹⁴ this commutation relation implies that the $\hat{T}_n|E_0\rangle$ are eigenstates with eigenvalues $E_0 - anF$. The form of the localized Wannier-Stark states for the long range hopping of Eq. (9) is shown in Fig. 3 (stars). The other wave function (circles) is discussed when we return to the discussion of the harmonic potential.

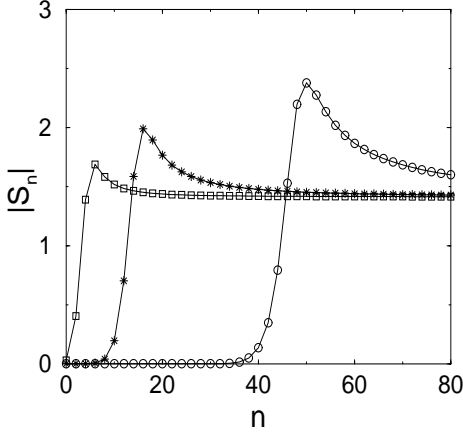


FIG. 2. Absolute value of the overlap $S_n \equiv \sum_m (-1)^m \psi_m^{(n)}$ which determines the deviation from the CCR as a function of the quantum number n for the even parity states, and different values of c : $c = 1$ squares, $c = 0.1$ stars and $c = 0.01$ circles.

We next examine if the CCR assumption is of any use for the understanding of the *time evolution* in the linear potential. The equations of motion for the Heisenberg operators $\hat{x}(t) \equiv e^{iHt}\hat{x}e^{-iHt}$ and $\hat{k}(t)$ close if the CCR are assumed and yield $\hat{k}(t)_{\text{CCR}} = \hat{k} + Ft\hat{1}$ as well as $\hat{x}(t)_{\text{CCR}} = \hat{x} + \hat{k}t + \hat{1}Ft^2/2$. Obviously the result for $\hat{k}(t)_{\text{CCR}}$ is incorrect as the operator \hat{k} defined in Eq. (3) is *bounded* and this property also has to hold for $\hat{k}(t)$. The result for the position operator using the CCR differs from the *exact* solution, which follows from $[\hat{x}, \hat{T}_n] = an\hat{T}_n$ and $[\hat{T}_n, H] = anF\hat{T}_n$ as

$$\hat{x}(t) = \hat{x} + \sum_{n>0} \left[t_n \hat{T}_n (e^{-ianFt} - 1) / F + H.c. \right]. \quad (10)$$

This shows that the exact solution is *periodic* in time. The particle undergoes so called “Bloch-oscillations”¹⁴.

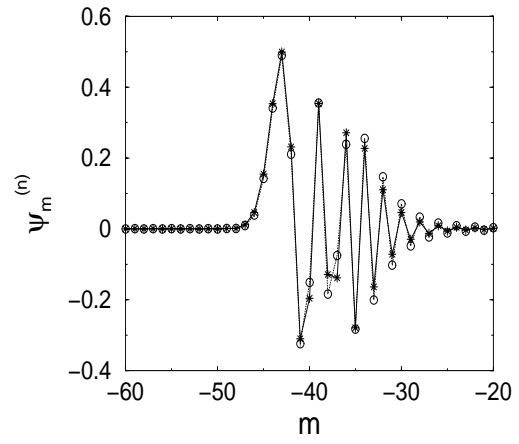


FIG. 3. The stars show the amplitudes $\sqrt{2}\psi_m$ of the Wannier-Stark eigenstate for a linear potential on a lattice with $F = 0.4$ localized around the site $m = -41$. The circles show the amplitudes ψ_m of the even eigenstate of the harmonic potential with $c = 0.01$ localized around the same site.

The two results are compared in Fig. 4 for two Gaussian wave packets ($\psi_n(t=0) \sim \exp[-b(n-n_0)^2]$) with the same location but different widths as initial states.

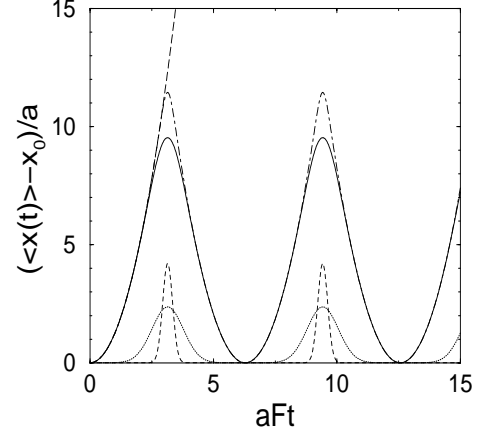


FIG. 4. The full curve ($b = 0.2$) and the dashed-dotted ($b = 0.02$) curve show the periodic Bloch oscillations in a linear potential ($F = 0.4$). The long dashed curve shows the result from assuming the CCR. In order to understand why this approximation fails qualitatively when approaching the time $\pi/(aF)$ the time dependent overlaps $|S_{\psi(t)}|$ (see text) are shown as the dotted ($b = 0.2$) and dashed curves ($b = 0.02$).

If the initial wave packet extends over many lattice sites the CCR assumption yields an excellent approximation for times less than $\pi/(aF)$. At this time the turning point is reached in the exact solution. Approaching this time the overlap $|S_{\psi(t)}| \equiv |\sum_n (-1)^n \psi_n(t)|$, also shown in Fig. 4, becomes large and the CCR assumption breaks down and yields a *qualitatively* wrong long time behaviour

with free acceleration as in the continuum. It should be pointed out that for a *linear potential* using a 2π -periodic function of $a\hat{k}$ for the kinetic energy, like e.g. the nearest neighbour hopping form $(\hat{1} - \cos a\hat{k})/a^2$ the CCR result for $\hat{x}(t)$ accidentally agrees with the exact solution. This is related to the fact mentioned earlier that the wrong use of the CCR yields the exact commutation relation $[\hat{x}, e^{-ina\hat{k}}] = ana e^{-ina\hat{k}}$ for integer n .

After this discussion of the linear potential we can return to the harmonic potential and explain its properties in the regime where the CCR assumption breaks down.

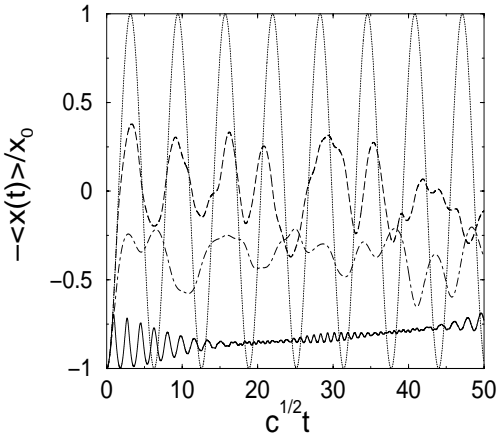


FIG. 5. Average position of initially Gaussian wave packets ($b=0.2$) centered at $x_0 = -n_0a$ in a harmonic potential ($c = 0.01$) as a function of \sqrt{ct} . For $n_0 = 20$ (dotted curve) the motion is harmonic as predicted by the CCR. For $n_0 = 30$ (dashed curve) many different excitation energies contribute and the motion is no longer harmonic. For $n_0 = 40$ (full curve) the time scale is too short to show the slow oscillation towards n_0a and back. The dashed-dotted curve is for the case of nearest neighbour hopping and $n_0 = 20$.

The almost degeneracy of pairs of eigenvalues shown in the upper right corner of Fig. 1 can now easily be explained. As shown in Fig. 3 (circles) the eigenstates for large enough quantum numbers are just even and odd states which (apart from a factor $\sqrt{2}$) almost look like the Wannier-Stark state which one obtains when the harmonic potential is linearized locally. The bonding-antibonding splitting decreases exponentially with the distance of the the right and left part of the eigenfunctions. This leads to a very slow component in the time evolution of the position operator shown in Fig. 5. For the same potential the time evolution strongly depends on the initial position $x_0 = -n_0a$ of the wave packet. For sufficiently small values of n_0 the expectation value $\langle \hat{x}(t) \rangle$ is to a very good approximation given by a cosine function as predicted by assuming the CCR. For $n_0 = 30$ many different frequencies contribute and lead to clear deviations from harmonic motion (dashed curve). For $n_0 = 40$ the initial state has strong overlap with eigenstates for which the bonding-antibonding splitting is al-

ready rather small and the slow oscillation towards an_0 cannot be seen in the figure. Only in the very short time limit the CCR result for expectation value is useful. The fact that the deviations get more pronounced by *increasing* n_0 is opposite to what is widely believed¹¹ but is obvious from Fig.1. One obtains qualitatively similar results if the long range hopping is replaced by nearest neighbour hopping, i.e. $\hat{k}^2/2 \rightarrow (\hat{1} - \cos a\hat{k})/a^2$ (see dashed-dotted curve in Fig. 5), which corresponds to the Josephson Hamiltonian. The two regimes indicated in Fig. 1 correspond to the Josephson and the Fock regime for this Hamiltonian¹¹. In the latter regime assuming the CCR must certainly fail for the long time dynamics.

In this paper we have shown that the fact that a canonical operator which is conjugate to the position operator on the lattice can be defined on a *dense set* of the Hilbert space is of very restricted use in practical applications. This is an indication that one has to be extremely careful in similar use of the particle number-phase CCR in fields like interacting electrons in one dimension⁴⁻⁶ and the Josephson effect¹¹.

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